

Problems and Paradoxes in High-dimensional Data

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Outline

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Sources of high-dimensional data

- **Biotech:** DNA microarrays, proteomics, transcriptomics etc.
- **Images / video:** medical, astrophysics, surveillance
- **Consumer preferences:** books, movie, music recommendation
- etc.

Examples

240p image $\sim 100,000$ pixels, 3 color bandwidth $p \approx 300,000$



Paradoxes

Volume of an n-D ball

- What's the volume of a circle with radius r ?
- πr^2
- What's the volume of a ball with radius r ?
- $\frac{4}{3}\pi r^3$

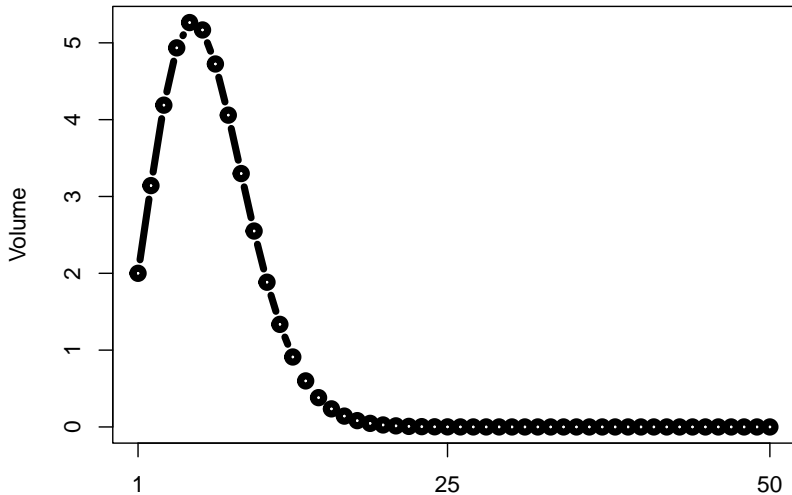
Volume of p -dimensional ball with radius $r > 0$

$$V(p; r) = \frac{1}{\Gamma(p/2 + 1)} \pi^{p/2} r^p \quad (1)$$

Does the volume get bigger or smaller as we increase p ?

Or more generally, how does the volume behave?

The volume



Where is the mass concentrated?

We've noticed that the volume of a p -dimensional ball tends to 0 as p increases, then naturally we might ask:

Where is the mass concentrated?

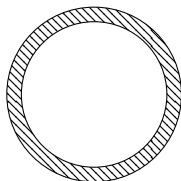
Where is the mass concentrated?

Consider the volume in the crust, i.e. the volume

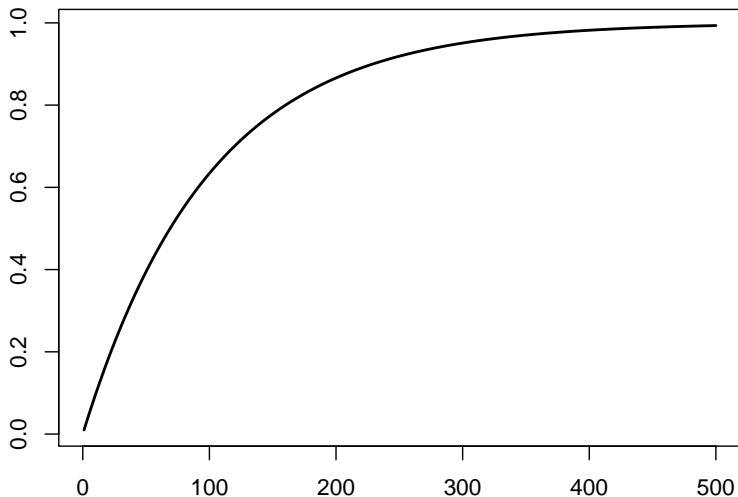
$$C(p; r) = V(p; r) - V(p; 0.99r) \quad (2)$$

Then the volume in the crust as a fraction of the total volume, i.e.

$$\frac{C(p; r)}{V(p; r)} = 1 - 0.99^p \quad (3)$$



Where is the mass concentrated?



So far...

Recap

- The volume of p -dimensional balls tends to 0
- The crust contains nearly all the mass

The lesson in all this is, we must be careful with our **geometric intuition** of high-dimensional spaces!

Paradoxes

There are many more counter-intuitive examples in high-dimensional spaces, to list a few

- Most of the mass of a standard Gaussian is in the tail!
- Rare events may not actually be that rare

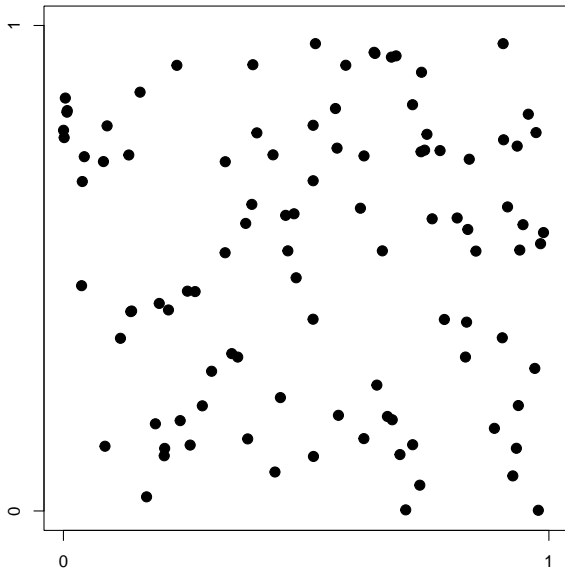
Problems

Data get far apart fast

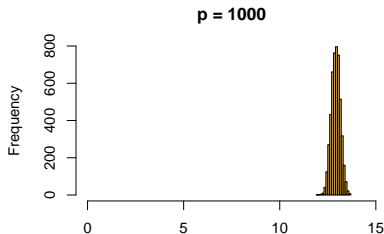
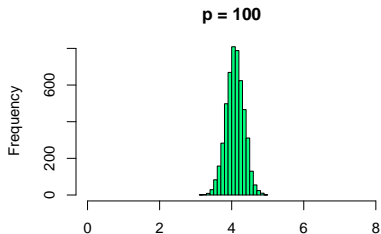
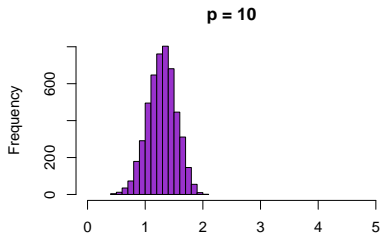
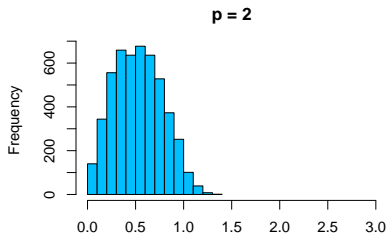
Suppose we have data uniformly distributed on a 2-D grid, 10-D grid, 100-D grid or 1000-D grid.

What's the average (euclidean) distance between points?

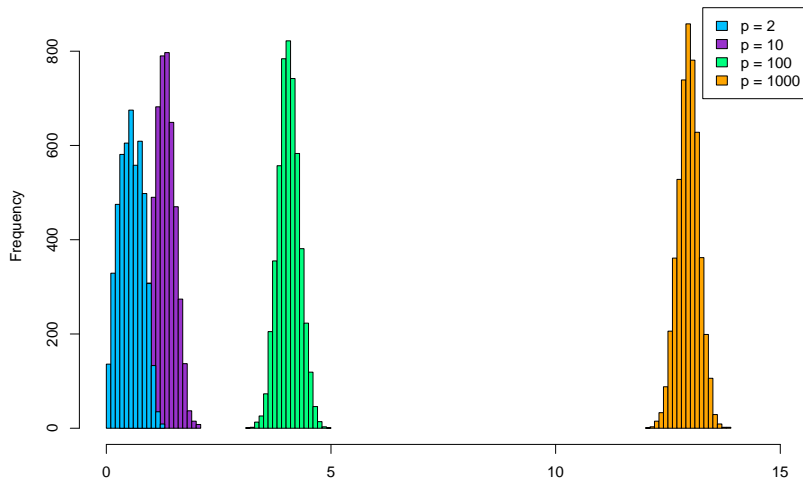
2D Case



What's the average distance?



What's the average distance?



What does this mean?

Distances between points

- The minimal distance between two points increases
- All points are a similar distance from the others
- The notion of nearest point vanishes

Some more problems

High-dimensional spaces are immense:

- **Vast**, data points can be isolated in the immensity
- **Small changes add up fast**. Many small fluctuations in different directions can produce a large global fluctuation
- **Computation** suffers

A practical example

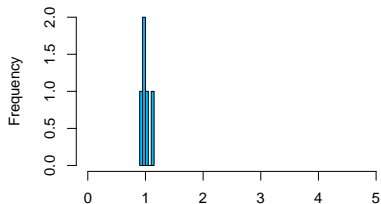
PCA relies on the estimation of the covariance matrix Σ .

Let's suppose we have some data generated iid from $\text{Normal}(0, I_p)$, where I_p is the $p \times p$ identity.

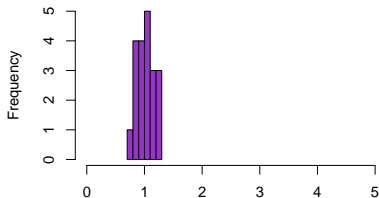
How well is Σ estimated as p grows?

To see how well we're doing we're going to compare the eigenvalues of the estimated covariance matrices to that of the true covariance matrix (I_p), we let $n = 1000$ and let $p = 5, 20, 250, 500$.

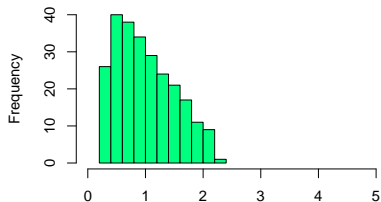
p = 5



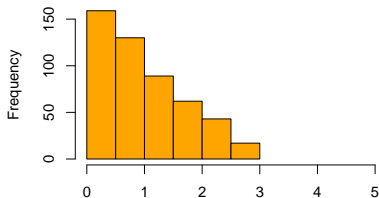
p = 20



p = 250



p = 500



PCA, main message

The empirical covariance is a very poor approximation of the covariance I_p in this setting.

In turn, downstream use of the covariance matrix (e.g. in PCA) can lead to spurious results.

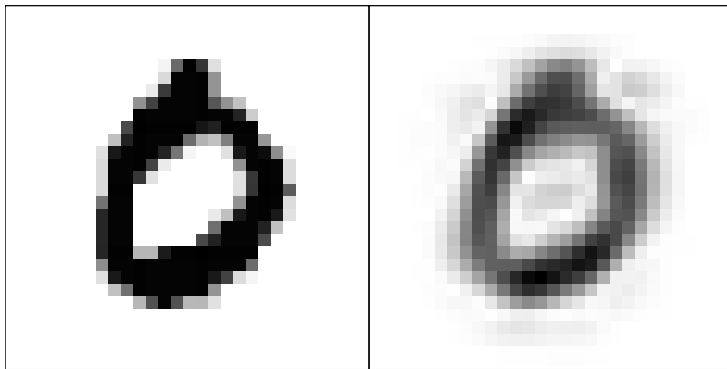
Silver lining

In many settings data is often much more low-dimensional and not uniformly spread!

- Images have structures
- Biological systems are strongly regulated
- Consumption reflects some social structures
- etc.

PCA on MNIST

Reconstructing the MNIST digits from the first 25 PCs



Overall, we **need to be careful** when analyzing high-dimensional data

Methods that can identify relevant structures or **incorporate the knowledge that these spaces are often sparse** generally outperform traditional methods.

Reference I

- [Gir21] Christophe Giraud. *Introduction to High-Dimensional Statistics*. Chapman and Hall/CRC, Aug. 2021.